The onset of jamming as the sudden emergence of an infinite k-core cluster

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A theory is constructed to describe the zero-temperature jamming transition of repulsive soft spheres as the density is increased. Local mechanical stability imposes a constraint on the minimum number of bonds per particle; we argue that this constraint suggests an analogy to k-core percolation. The latter model can be solved exactly on the Bethe lattice, and the resulting transition has a mixed first-order/continuous character reminiscent of the jamming transition. In particular, the exponents characterizing the continuous parts of both transitions appear to be the same. Finally, numerical simulations suggest that in finite dimensions the k-core transition can be discontinuous with a nontrivial diverging correlation length.

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Understanding a continuous phase transition is tantamount to determining the universality class to which it belongs. In contrast, understanding the nature of a discontinuous change of phase requires a detailed study of the system at hand. Under normal circumstances [1], the two categories are mutually exclusive. However, there are a few examples of continuous transitions that exhibit characteristics of first-order transitions [2, 3, 4, 5, 6, 7, 8, 9, 10]. In this Letter, we will present arguments that the jamming transition in sphere packings[11, 12, 13] belongs to this class and can genuinely be described as both continuous and discontinuous. Indeed, we will identify the minimal physics needed to capture the nature of the transition by analogy to the k-core percolation model, and show by exact calculation that the latter model has a true mixed transition of this type with similar exponents at the level of mean-field theory. We also present numerical evidence that k-core models can still exhibit mixed transitions in finite dimensions. We remark that, starting from a different vantage point, Toninelli, *et al.* [14] have arrived at a model of the k-core type and have reached similar conclusions about the nature of the transition in their studies of kinetically-constrained models.

Numerical studies [11, 12, 13] of sphere packings at zero temperature suggest that there is a packing density ϕ_c (Point J) where the onset of jamming is truly sharp; i.e. the static bulk and shear moduli vanish for $\phi \leq \phi_c$ and are nonzero for $\phi > \phi_c$. This transition exists for spheres that repel when they overlap and otherwise do not interact. For small ϕ, particles easily arrange themselves so as not to overlap with any other particle and hence the total potential energy is $V \equiv 0$. As ϕ is increased, there is a particular value of ϕ_c above which the particles can no longer "avoid" each other and V becomes nonzero. The average coordination number (the average number of overlapping neighbors per particle) is $Z = 0$ for $\phi < \phi_c$. As ϕ approaches ϕ_c from above, however, the behavior is very different: $< Z > \approx Z_c + Z_0(\phi - \phi_c)^{\beta}$, where $\beta = 0.49 \pm 0.04$ [12]. Moreover, the singular part of the shear modulus vanishes with the exponent $\gamma = 0.48 \pm 0.05$ [12] and recent simulations by Silbert, *et al.* [13] find a diverging length scale exponent $\nu = 0.24 \pm 0.03$ [13, 15].

These numerical results imply that the transition at Point J has characteristics of both types: certainly there is a discontinuity in the average coordination number, $\langle Z \rangle$, but as the transition is approached from the ordered (jammed) phase, it exhibits the typical singularities associated with continuous transitions; $\langle Z \rangle$ tends to its limiting value with a nontrivial power-law and there are divergent length scales.

We will now present arguments that the Point J transition is indeed a mixed transition, many aspects of which can properly be understood by analogy to a relatively simple model called "k-core percolation" (sometimes also called "bootstrap percolation" [16]). Let us start with an informal discussion of the essentials of the jamming model. Clearly, a jammed packing of spheres at $T = 0$ must be mechanically stable. For a sphere in d dimensions to be locally stable, it must have interactions (*i. e.* overlap) with at least $d+1$ neighboring spheres [17]. Evidently, spheres with fewer than $d+1$ overlapping neighbors do not contribute to the formation of a jammed structure and thus are *irrelevant*. Thus we may envision the mechanics for a system below the jamming threshold density as its energy is lowered towards the minimum: although large clusters of overlapping particles may happen to form, those at the boundary of the cluster are unstable and will move away, further lowering the energy. This in turn exposes secondary particles, who are in turn forced to move away, and so forth until the cluster dissolves. At

high density the situation is more complicated. However, it is still true that all particles that *do* contribute to the jammed structure must have at least $d+1$ overlapping neighbors that are not "irrelevant", and each of these overlapping neighbors must have at least $d+1$ overlapping neighbors that are not irrelevant, and so on. In other words, only particles that survive this entire hierarchy of irrelevance can contribute to the jammed structure.

These considerations are suggestive of the k-core percolation model, defined as follows. Consider a regular lattice of coordination number $Z_{\max}$ and some integer k with $2 \leq k < Z_{\max}$. Initially, sites are independently occupied with probability p. In the first stage, all occupied sites with fewer than k neighboring occupied sites are eliminated. Then, this decimation process is applied to the surviving occupied sites, and so on, until all surviving sites (if any) have at least k surviving neighbors. Thus, at the end of this process, every surviving site has at least k neighbors, all of whom in turn have at least k neighbors, etc. The surviving sites are called the k-core and phases of the model are determined by the presence or absence of an infinite cluster of these survivors.

The overall analogy between the two models is self-evident. The initiating density p corresponds the the packing fraction ϕ, k corresponds to $d+1$ and $Z_{\max}$ to the so-called *kissing number*, that is the maximum number of equivalent hyperspheres in d dimensions that can touch a central one without overlaps. (In $d=2$, $Z_{\max}=6$, and in $d=3$, $Z_{\max}=12$.)

In the mean-field theory of k-core percolation, i.e. the Bethe lattice and infinite-range complete graph models, it is well-established that the order parameter undergoes a discontinuous jump at threshold [16, 18], accompanied by a square-root singularity [16, 18, 19]. However, the fact that the latter was indicative of a *critical phenomenon* has heretofore been underemphasized; in particular, a divergent length scale had not been identified. Below we will show that, at least on the Bethe lattice, there is indeed critical behavior in the sense of a diverging susceptibility and correlation length and the various exponents are in (rather dramatic) agreement with their counterparts in the Point J simulations.

The k-core percolation model can be solved exactly on the Bethe lattice. We begin by considering the half-space Bethe lattice, for which we derive recursion relations for quantities at level $n+1$ in terms of quantities at level n. All occupied sites at level 0 of the half-space Bethe lattice belong to what we call the "deep core." We keep track of two quantities, the probability of belonging to the deep core at level $n+1$, $\Upsilon^{\rm HS}_{n+1}$, which requires the site at level $n+1$ to have at least k neighbors at level n that belong to either the deep core or to what we call the "corona." To be in the corona at level $n+1$, a site must have *exactly* $k-1$ neighbors at level n that belong to the deep core or the corona. We denote by $\Phi^{\rm HS}_{n+1}$ the probability of belonging to the corona at level $n+1$, and by $\Gamma^{\rm HS}_{n+1} \equiv \Upsilon^{\rm HS}_{n+1} + \Phi^{\rm HS}_{n+1}$ the probability of belonging to either the deep core or the corona. The deep core will necessarily be part of the k-core; we need to keep track of the corona because when two half-spaces are glued together to form the full Bethe lattice, corona can be converted to k-core. The recursion relation is

$$\begin{aligned}\Gamma^{\rm HS}_{n+1} &= p \sum_{l=k-1}^{Z_{\max}-1} \binom{Z_{\max}-1}{l} (\Gamma^{\rm HS}_n)^l (1-\Gamma^{\rm HS}_n)^{Z\max-1-l} \\ &\equiv p\Pi^{Z_{\max}}_{k-1}(\Gamma^{\rm HS}_n). \end{aligned} \tag{1}$$

In the limit of large n, $\Gamma^{\rm HS}_n = \Gamma^{\rm HS}_{n+1} \equiv \Gamma^{\rm HS}$. Clearly, $\Gamma^{\rm HS}=0$ is always a solution. However, there can be a nontrivial solution for p exceeding some p_c. For $k \geq 3$ [16, 19]

$$\Gamma^{\rm HS} \sim a + b(p-p_c)^{1/2} \tag{2}$$

At the transition, the curve $p\Pi_{k-1}(\Gamma^{\rm HS})$ is just tangent to $\Gamma^{\rm HS}$, *i. e.* $p_c\Pi'_{k-1}(\Gamma^{\rm HS})=1$.

The average coordination number, susceptibility and correlation length exponents, which are needed for the comparison to sphere packings, must be calculated on the full Bethe lattice, obtained by connecting two half-space lattices. The resulting probability of belonging to the k-core, K, is given by $K = \Upsilon^{\rm HS} + \Phi^{\rm HS}\Gamma^{\rm HS}$. This has the same behavior as $\Gamma^{\rm HS}$ in Eq. 2. The average number of occupied neighboring sites per occupied site (*i. .e.* the average coordination number) also behaves in the same fashion as $\Gamma^{\rm HS}$ (Eq. 2). It jumps from zero for $p<p_c$ to $\langle Z\rangle \approx Z_c + Z_0(p-p_c)^{1/2}$ for $p>p_c$, in excellent agreement with the numerical results for sphere packings [12].

The susceptibility is the sum of correlation functions, $\tau_{\ell,m}$, connecting levels ℓ and m of the Bethe lattice, and has the form $\chi = \sum_n (Z_{\max}-1)^n \tau_{0,n}$. We consider two different correlation functions: $\tau^{\#}_{0,n}$ represents the probability that both level 0 and level n are connected to the deep core, while $\tau^{*}_{0,n}$ represents the probability that levels 0 and n are connected to each other via the corona [20]. This latter probability can be derived by considering the chain of sites connecting a given site at level 0 to a site at level n. To belong to the corona, each site along the chain must be occupied and have exactly k neighbors (including the two adjacent sites along the chain) connected to the deep core or corona. The corresponding probability for each site is $\Theta = p\binom{Z_{\max}-2}{k-2}(\Gamma^{\rm HS})^{k-2}(1-\Gamma^{\rm HS})^{Z_{\max}-k}$. The final probability $\tau^{*}_{0,n}$ therefore scales as Θ^n. When this is summed over n, it yields a susceptibility exponent of $\gamma^*=1/2$. By somewhat more complicated reasoning, the dominant contribution to $\tau^{\#}_{0,n}$ scales as $n\Theta^n$; this leads to $\gamma^{\#}=1$. Note that $\tau^{*}_{0,n}$ measures the size of the corona, which is the region that can be converted into k-core or not, depending on the state of only one site. This is the source of cooperativity underlying the transition.

Another way to compute a susceptibility is to calculate the response to a perturbation; in the case of percolation,

this corresponds to the addition of low-probability "short routes to the infinite cluster." In our system we have done this in two ways: first by providing a small fraction of additional random sites with $k-2$ occupied neighbors that are connected directly to the deep core plus corona, and secondly by declaring a small fraction of sites to be in the deep core plus corona regardless of their connectivity. Both prescriptions yield $\gamma^* = 1/2$, as well as a "magnetic field" exponent of $\delta^* = 2$.

The correlation length corresponding to *both* susceptibility exponents diverges with the exponent $\nu^* = 1/4$ (although there is a logarthmic difference between the two). We use the usual embedding of a Bethe lattice in Euclidean space [21] to arrive at this result. One would expect the usual mean field relation $\nu = \gamma/2$ to hold; the exponent $\gamma^{\#} = 1$ may be an artifact of the Bethe lattice. However, we also obtain $\nu^{\#} = 1/2$ by looking at how quickly the order parameter approaches its bulk value as a function of distance from the boundary.

The exponents $\beta = 1/2$, $\gamma^* = 1/2$, and $\nu^* = 1/4$ are in excellent agreement with numerical simulations of particle packings near Point J. However, these simulations are carried out in 2 and 3 dimensions while the k-core calculations correspond to infinite dimensions (the mean-field limit). This raises the question of whether the mixed nature of the k-core transition can survive in finite dimensions. Most studies have focused on particularly simple systems such as the $2d$ square and triangular lattices [22], some $3d$ cubic lattices [23] and hypercubic lattices [9]. For these simple systems, the transition falls into one of two categories: Either the transition is continuous or it does not occur until $p = 1$. Systems that exhibit continuous transitions all contain self-sustaining clusters, *i. e.* clusters that are finite and yet survive the decimation process. For example, for $k = 3$ on the $2d$ triangular lattice, the smallest self-sustaining cluster is a fully-occupied hexagon and the k-core transition appears to correspond to ordinary percolation of these hexagons [22]. Systems that fail to exhibit a transition below $p = 1$ apparently contain "unstable voids" [9, 24, 25] that lead to decimation of the entire population whenever $p < 1$.

We regard percolation of self-sustaining clusters and unstable voids as "artifacts" of simple k-core models. Indeed, for jammed sphere packings these two effects cannot arise. First, self-sustaining clusters of overlapping particles are forbidden due to the repulsive nature of the interactions between particles. Likewise, voids (i.e. collections of floaters, or particles with no overlapping neighbors) cannot grow because of the force constraints and because floaters can shift around, but cannot actually disappear. To see this, consider the interface between a void and the surrounding sea of particles with at least k overlapping neighbors. For a sufficiently large void, a particle on the boundary with at least k overlapping neighbors will inevitably experience a nonzero net force into the void, since floaters provide no compensating force. Thus, large voids will shrink away; they will not grow. To capture some of this physics, we have introduced a 3-core model with '"force-balance" on the square lattice [26]. Potential neighbors are located within a 5x5 square centered upon the site of interest; thus, $Z_{max} = 24$. To survive decimation, any given site must have at least 3 occupied neighbors and if there is at least one occupied neighbor to the right of the site of interest, there must be at least one occupied neighbor to its left and vice versa. Similarly, if there is at least one occupied neighbor above the site of interest, there must be at least one occupied neighbor below and vice versa.

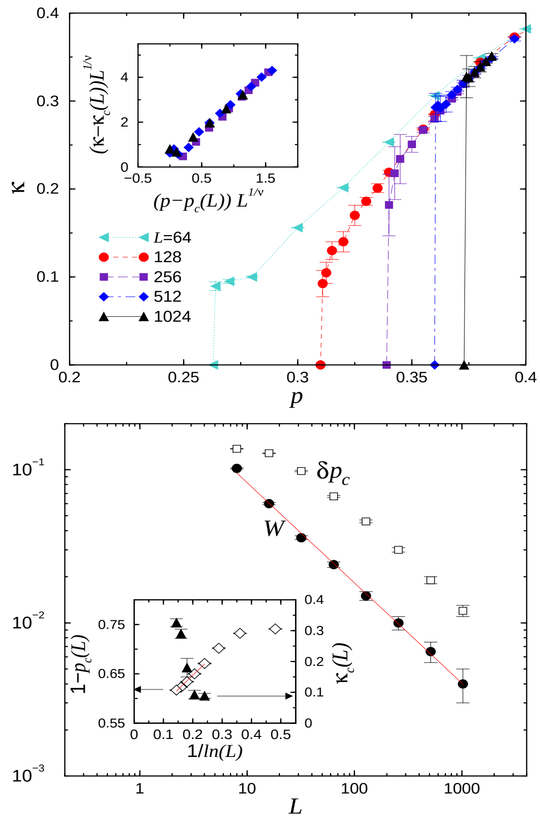

FIG. 1: Top: The order parameter $\kappa(p)$ for different system lengths L. Inset: Scaling collapse for $L = 256$ and larger. Bottom: Log-log plot of the width of the transition, W (solid circles) and the critical point shift δp_c (open squares) as a function of L with a power-law fit (line) with $\nu = 1.52(2)$ for W and $\nu = 1.53(1)$ for δp_c. The inset shows the jump κ_c, remains nonzero (solid triangles and right axis) and that p_c remains smaller than unity (open diamonds and left axis) as $L \to \infty$.

We have undertaken simulations of this 3-core model, and find evidence that the transition is discontinuous with a diverging correlation length. In Fig. 1a, the fraction of occupied sites in the spanning cluster, κ, is plotted as a function of p for different system lengths L. For each L we observe that κ jumps from zero to $\kappa_c(L)$ at some $p_c(L)$. For a continuous transition, the jump $\kappa_c(L)$ would

decrease with L and vanish as $L \to \infty$, but here $\kappa_c(L)$ *increases* with L. The size of the jump $\kappa_c(L)$ appears to approach a nonzero limiting value of 0.374(1) (solid triangles in inset to Fig. 1b). Furthermore, the transition point, $p_c(L)$ approaches $p_c = 0.396(1)$ for $L \to \infty$. To verify that unstable voids do not drive the transition to $p_c = 1$, we plot $1 - p_c(L)$ vs. $1/\ln L$ as open diamonds in the inset to Fig. 1b. We do not find linear behavior with a y-intercept of zero, as predicted for $p_c = 1$ [25].

We calculate the correlation length exponent from two different quantities (Fig. 1b): (1) the width of the transition defined by $W = p_+(L) - p_-(L)$, where $p_\pm(L)$ are defined as the values of p at which the probabilities of obtaining a spanning cluster are 0.25 and 0.75, respectively, and (2) the critical point shift $\delta p_c \equiv p_c - p_c(L)$. Both W and δp_c scale as $L^{-1/\nu}$ with $\nu = 1.52(2)$ and 1.53(1) respectively, as shown in Fig. 1b. This exponent leads to scaling collapse of the order parameter curves of Fig. 1a, as shown in the inset to Fig. 1a. Here, we assume the scaling form $\kappa(p, L) = \kappa_c(L) + L^{-\beta/\nu} f((p - p_c(L))L^{1/\nu})$, with $\beta = 1.0$ (for optimal collapse). For ordinary first-order transitions, finite-size scaling would predict a diverging length with an exponent of $1/d$ [27], corresponding to 0.5 in $d = 2$. We obtain an very different exponent, strongly suggesting a mixed transition. Analysis of a recently-proposed lattice model reaches a similar conclusion [14]. Furthermore, a recent $1/d$ expansion of pure k-core percolation suggests that the mixed nature of the mean field transition may survive in finite dimensions [28].

While k-core percolation appears to capture the minimal physics needed to explain the mixed transition found at Point J, it is not a complete description of jamming. This can already be seen by comparing the exponents observed for the mixed transition of the $d = 2$ 3-core model, $\beta \approx 1.0$ and $\nu \approx 1.5$, with those found in the $d = 2$ and $d = 3$ jamming simulations, $\beta = 0.49$ and $\nu = 0.24$. In fact, k-core models do not include a very important property of the jamming transition, namely isostaticity[17]. At Point J, the number of overlapping neighbors jumps from zero to $Z_c = 2d$ where d is the dimensionality. In k-core percolation, on the other hand, Z_c is not universal; it depends on k and $Z_{\max}$. We find that the global constraint of k-core percolation yields $Z_c > k$, even though the local constraint only requires k neighboring occupied sites per site.

Duxbury, *et al.*[29] have proposed that the closely-related problem of rigidity percolation can be mapped onto the k-core percolation problem in mean-field by imposing the constraint that the transition should occur when Z_c satisfies the isostatic condition. Thus in their formulation, the mean-field transition occurs above p_c, at some p_r at which Z_c reaches its isostatic value. They therefore obtain an isostatic, ordinary first-order transition, while k-core percolation yields a non-isostatic, mixed transition. Neither case properly applies to the jamming transition, which appears to be both mixed and isostatic [12, 13]. We note that a complementary theory by Wyart, *et al.* [30] starts with isostaticity at Point J and successfully describes the behavior of the density of vibrational modes and predicts a diverging length scale with exponent of 1/2, with much the same physical meaning as our $\nu^\# = 1/2$. In addition, a recent field theoretical approach also starts with isostaticity and appears to produce some of the same mean-field exponents that we find [32]. We speculate that a complete theory of jamming would exhibit the same mean-field exponents as k- core percolation, but different behavior in finite dimensions due to isostaticity; the latter effect suggests an upper critical dimension of two [30, 31].

We have argued that the physical constraint of requiring at least $k = d + 1$ overlapping neighbors per particle in zero-temperature sphere packings leads to a transition resembling the k-core percolation type. However, this analogy may have implications ranging beyond sphere packings to glassforming liquids. This connection is suggested by the set of exponents we find for mean-field k-core percolation, which is rare but has been seen in a few other models that are known to exhibit glassy dynamics as the temperature is lowered. These include the mode-coupling theory of glasses [34], mean-field theories of the p-component spin glass [5, 35] and kinetically-constrained spin models [7, 8, 9, 10]. For the latter models, this is no coincidence since they map onto k-core percolation and its variants [8, 9, 10]. Finally, we note that models such as the 3-SAT spin glass are also variants of k-core percolation. It can be shown that in mean field, the unfrustration-frustration transition has the same mixed character as in k-core percolation, suggesting that the 3-SAT spin glass may exhibit glassy dynamics.

It has been proposed [33, 36] that the behavior of many jamming systems, including glasses, suspensions, foams and granular materials, might be captured by "jamming phase diagrams," in the three-dimensional space of temperature T, applied shear stress σ, and packing density ϕ. In this space, the boundary separating jammed from unjammed behavior is a "surface" whose location is nebulous because it depends on the time-scale of the observations, and Point J lies underneath the jamming surface. Numerical simulation results [12, 13] suggest that the entire jamming surface of the jamming phase diagram is indeed controlled by Point J, the unique point where a sharp transition occurs. Here, we have argued that the physics near Point J is strongly suggestive of the k-core problem. The latter has a transition with unusual features that mirror corresponding features found at Point J: a mixed first–second order transition and the same exponents that characterize the continuous part. In contrast to earlier scenarios of the glass transition based on avoided critical points, either at nonzero temperature [37] or zero temperature [38, 39], the arguments of O'Hern, *et al.* [12] evidently suggest a scenario based on

an avoided *mixed* transition at Point J. On one hand, the first-order character of the transition may explain the presence of strong system-specific features such as the degree of fragility. On the other hand, the continuous component of the transition may explain the many ubiquitous features in the phenomenology of jamming [33].

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